Development of AMPYRE – A Dynamic Pyroprocess Model

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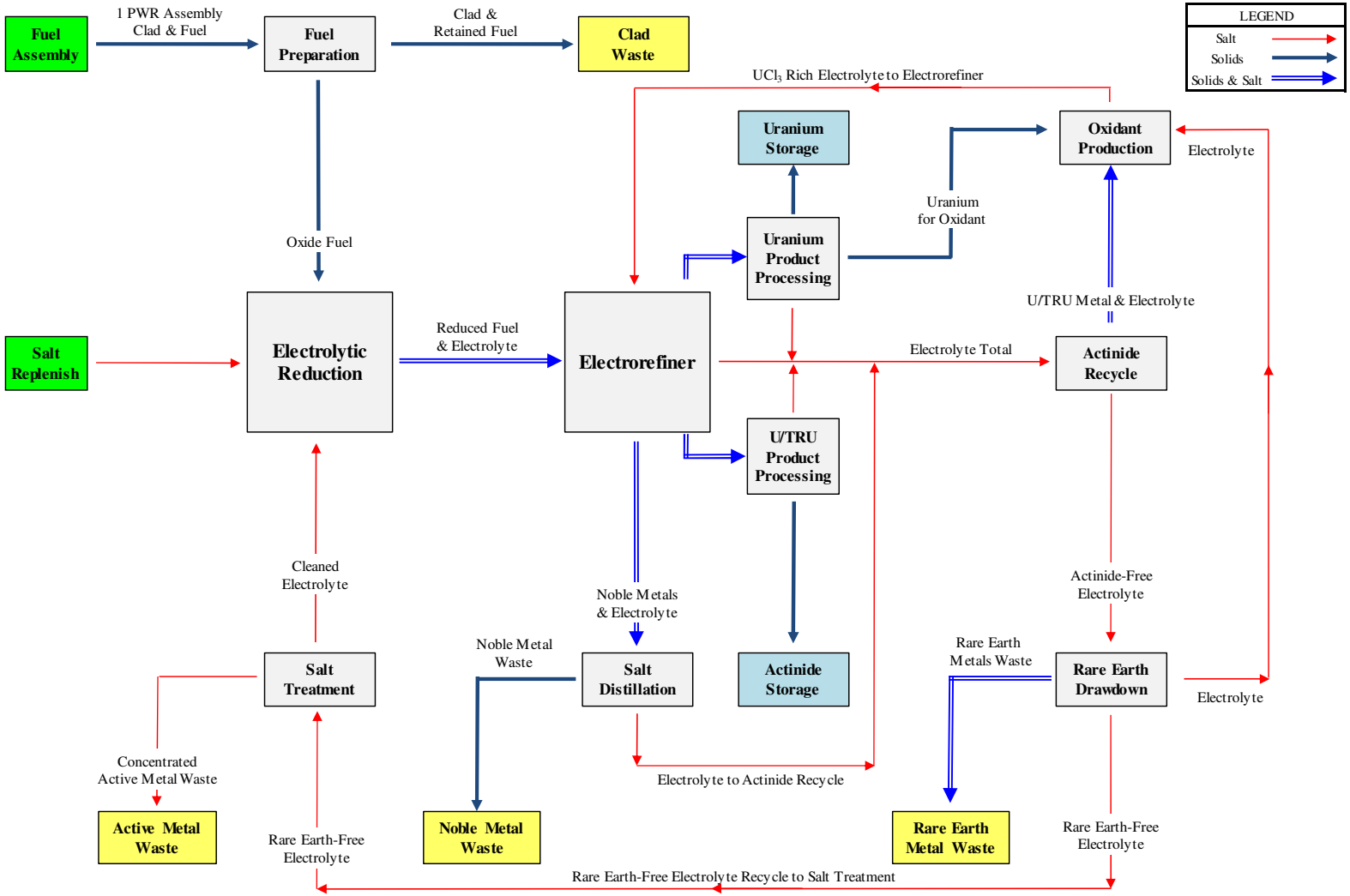
Development of Argonne Model for PYrochemical Recycling (AMPYRE)

- Mass-balance model of a complete electrochemical facility
  - User interface, calculations, and formatted output all programmed using Microsoft Excel with Excel VBA
- Unit operations of facility, with interdependency
  - Head end operations
  - U and U/TRU product collection
  - Salt recovery, treatment, and recycle
  - Wasteform fabrication
  - Predicts batch-wise evolution of salt and product compositions
  - Simple variables representing chemical behavior
    - Chemistry-based models being developed for anode and cathode subunits
- Can be used to explore
  - Effect of changing operating conditions or fuel composition
  - Impact of variations in inputs
  - Flowsheet option comparisons

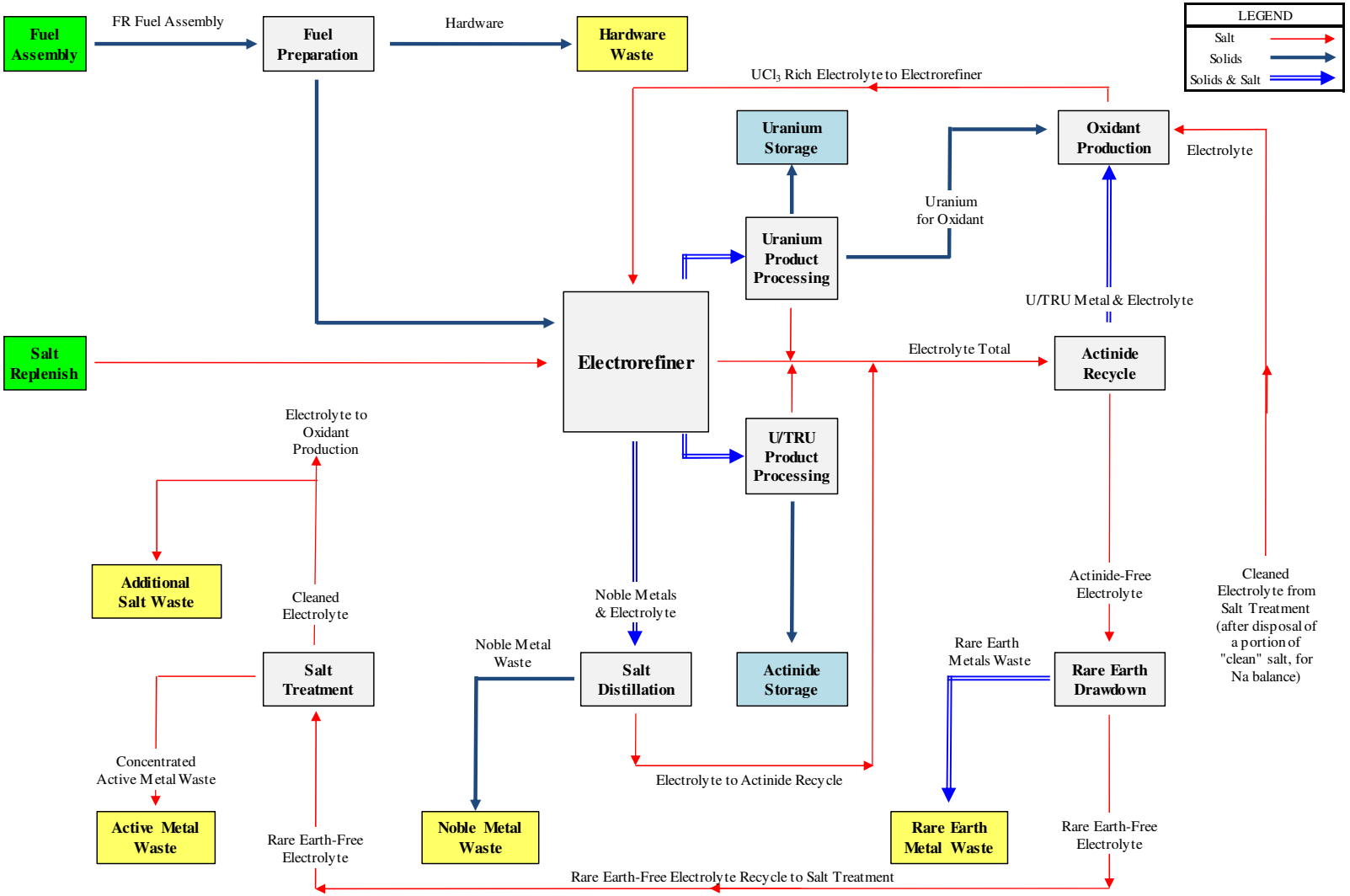
Key Features of A Fully-Integrated, Dynamic Pyrochemical Process Model

- Accurately models all separations steps in the process
  - Chemical separation & conversion steps (e.g. oxide reduction, electrorefining, actinide recovery, oxidant production, etc.)
  - Physical separation steps (U-product processing, U/TRU product processing)
  - Wasteform production (metal and ceramic wasteforms)
- Accurately tracks evolution of salt and product compositions as material moves through an electrochemical reprocessing facility
  - Material transfers of discrete batches of solids with solid adhered salt
  - Material transfers of molten salt
  - Batch and semi-continuous process operations
- Accurately handles transition from start-up to steady state
  - Not all process operations are performed initially (e.g. U/TRU deposition, actinide drawdown, rare earth drawdown, wasteform production)
  - Processes “turn on” when concentrations of key species in salt build up to target levels

Flowsheet for LWR Fuel

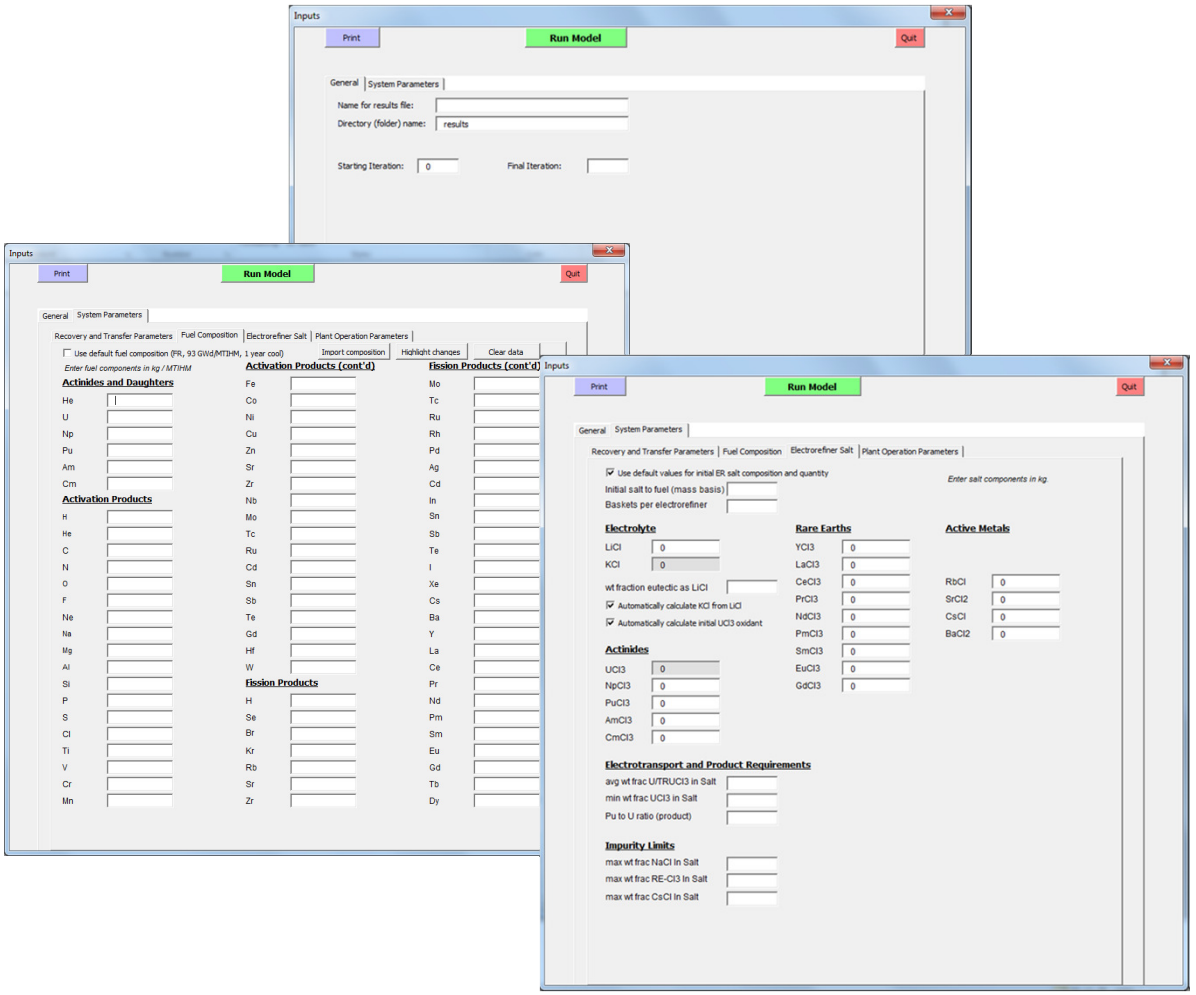


Flowsheet for Metal Fuel



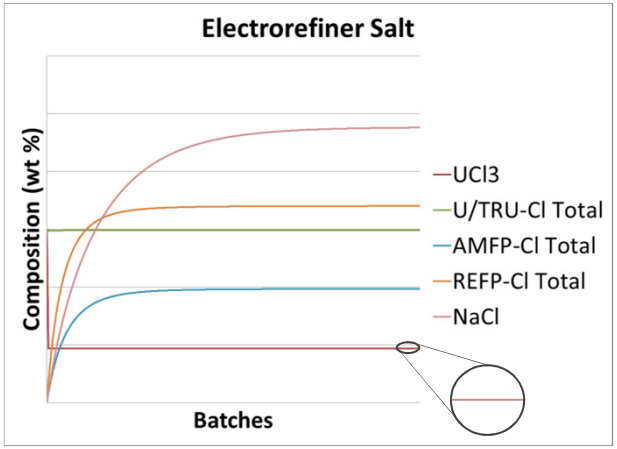
A User-Friendly Dynamic Model

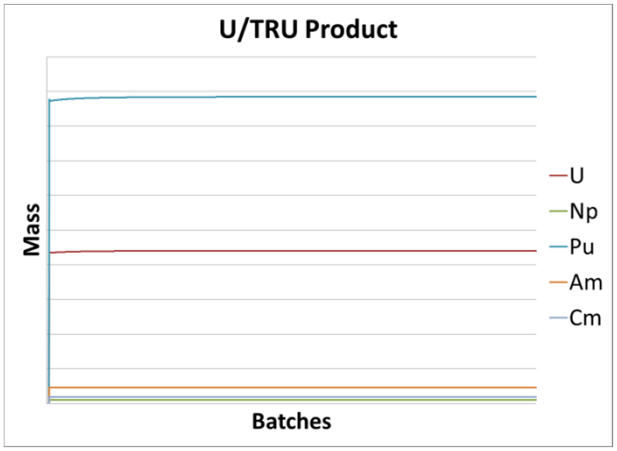
- Model was built using MS Excel and VBA
- Automated handling of operating changes and resumption of existing runs
- Revised code to handle variable inputs
- Import user-defined fuel composition from spreadsheet
- Expanded options for Cs/Sr recovery



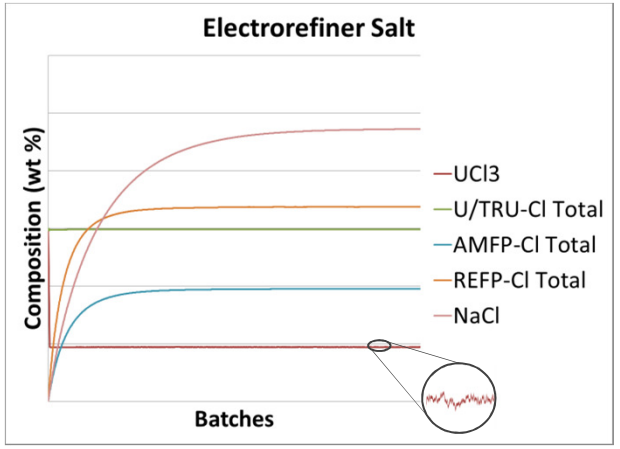
Sensitivity Analysis: Variation in Metal Fuel Composition Input

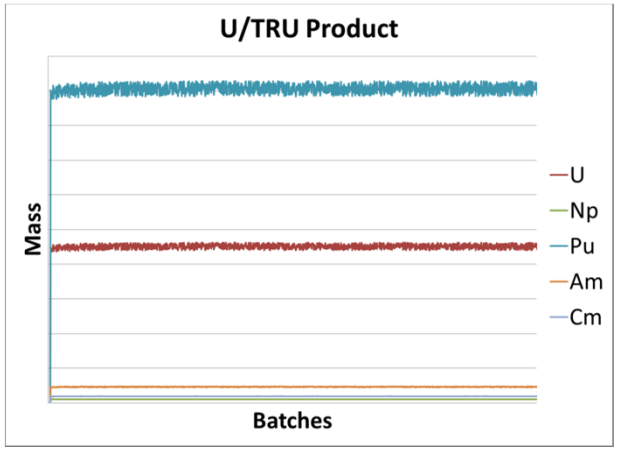
Constant Fuel Composition





Variation in Pu Content of Fuel

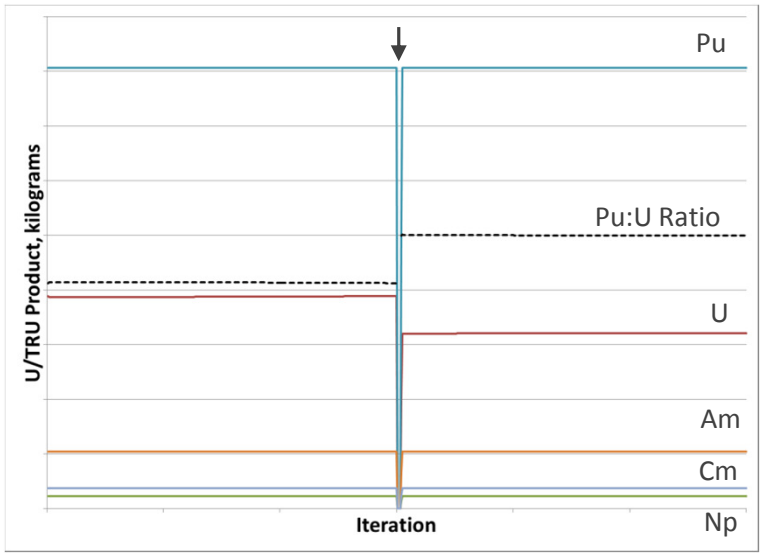




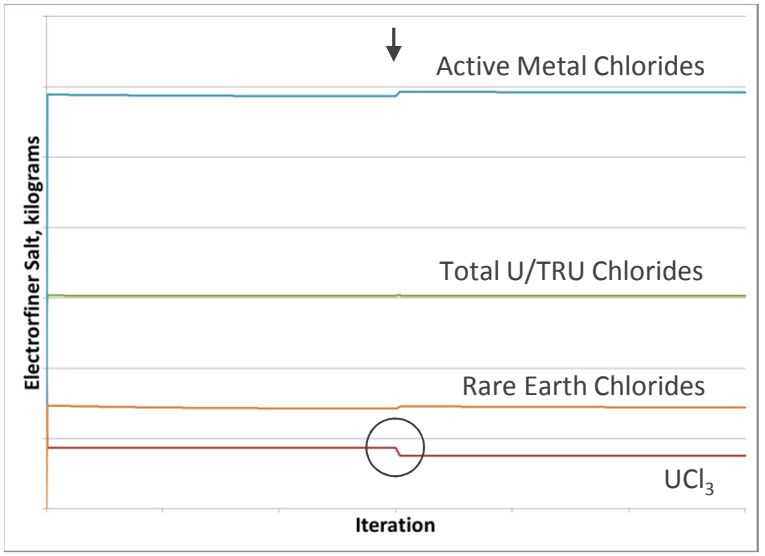
System Response to Changes

- Ability to adjust to operational changes

U/TRU Product



Electrorefiner Salt



- User interface can load previous results and resume calculation
- Predicting effect of operational changes is key to materials tracking

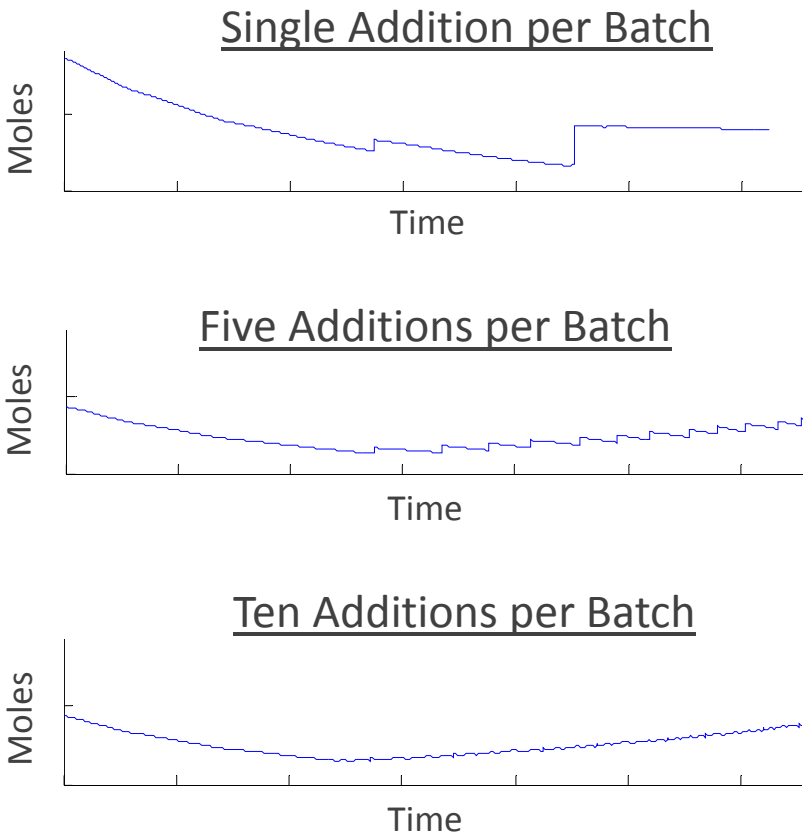
Development of Dynamic Electrorefiner Model (DyER)

- Time-dependent, current-based electrorefiner model
- Calculations in MATLAB®
- Electrochemical models of anode and cathode behavior
- Simplified approach to salt recycle
  - To be used in combination with mass-balance facility model
- Predicts time-dependent evolution of salt and product compositions from user-defined operating conditions:
  - Initial salt composition and fuel composition
  - Number of cathodes; anode and cathode surface area
  - Operation at constant voltage or constant current
  - Adjustable oxidant addition
  - Can be used to explore transient conditions in the electrorefiner
- Can be interfaced with AMPYRE

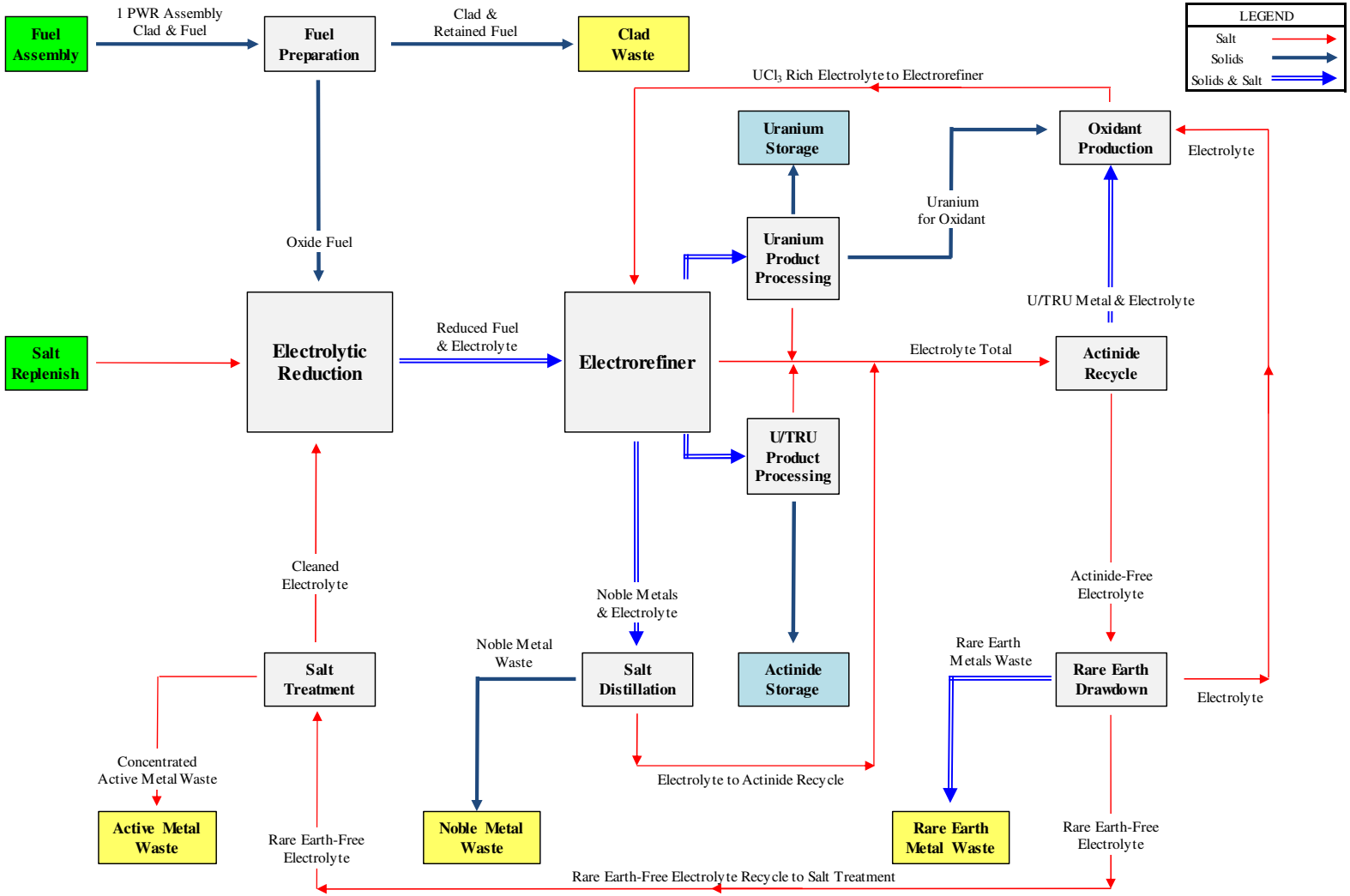
Example of Dynamic Electrorefiner (MATLAB) Model Results

- Effect of Method of Oxidant Addition
  - Processing multiple batches
  - Varying frequency of oxidant addition
    - Single addition per batch
    - Multiple additions per batch
    - Continuous addition of oxidant
  - Scale of observable response

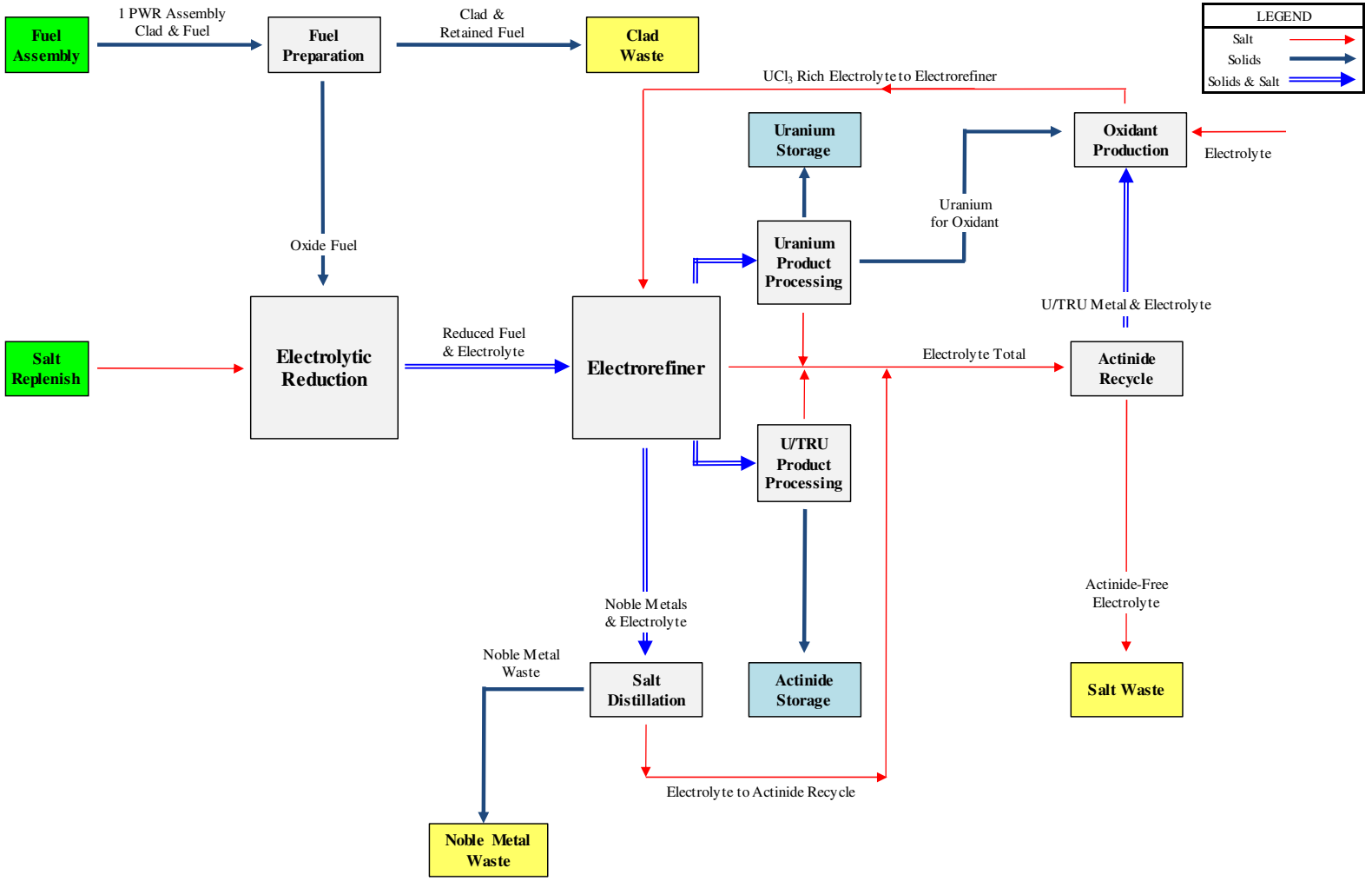
UCl_3 in Electrorefiner Salt



Flowsheet with Salt Recycle

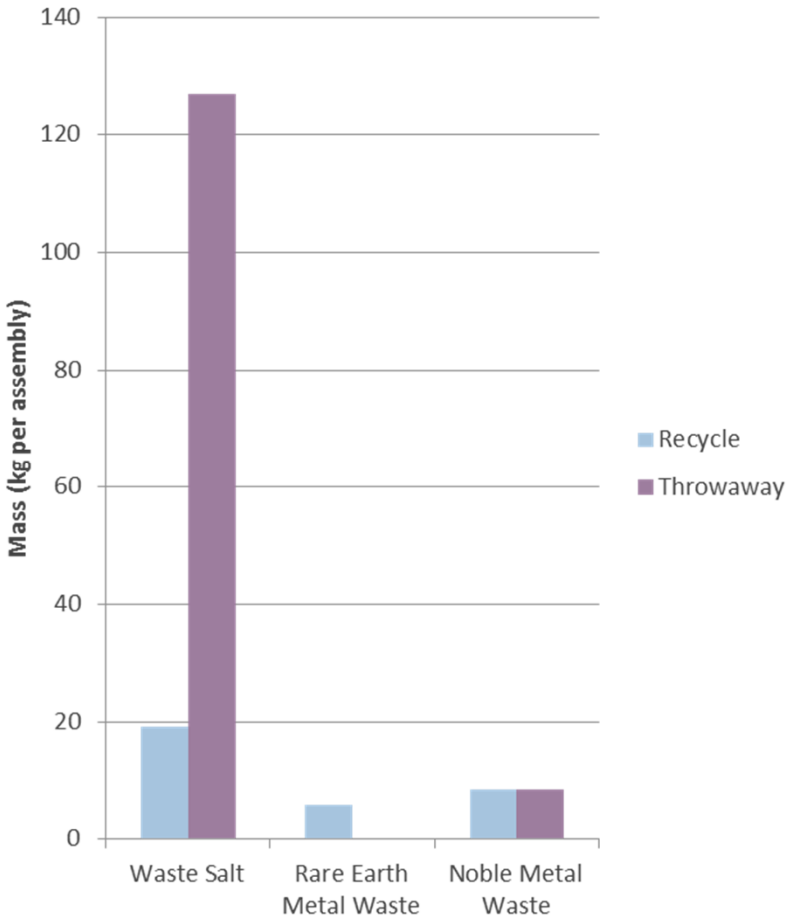


Flowsheet with Direct Throwaway



Using AMPYRE to Evaluate Flowsheet Options (Oxide Fuel)

- Comparison of salt handling options
  - Recycle loop to remove rare earth and active metal fission products
  - Direct throwaway of electrorefiner salt following recovery of U/TRU
- Impact on waste



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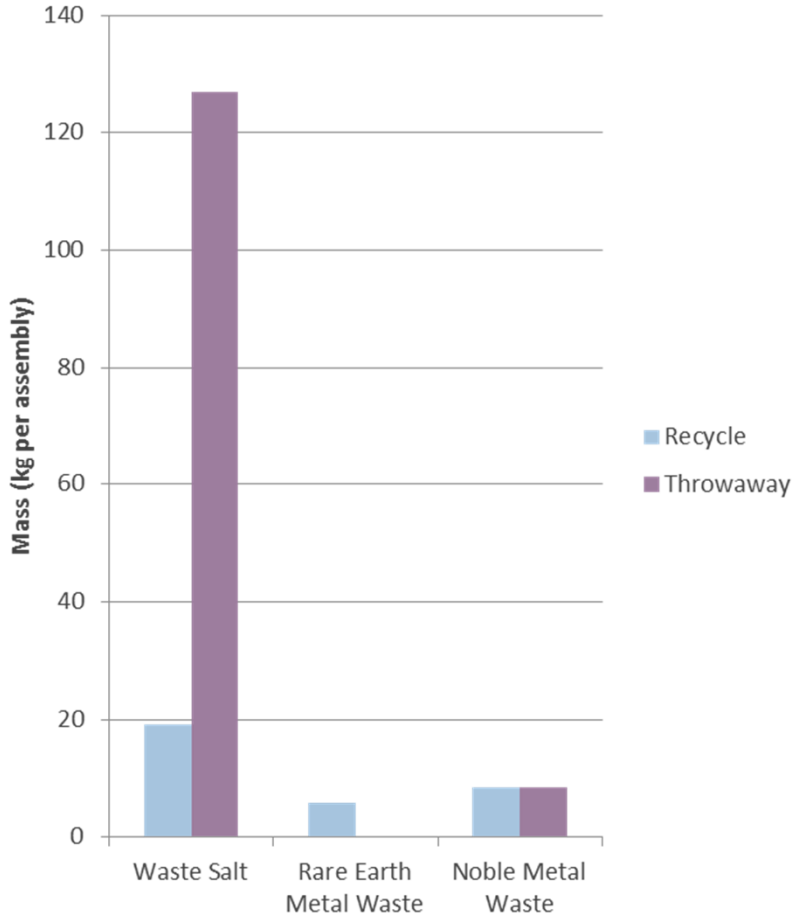
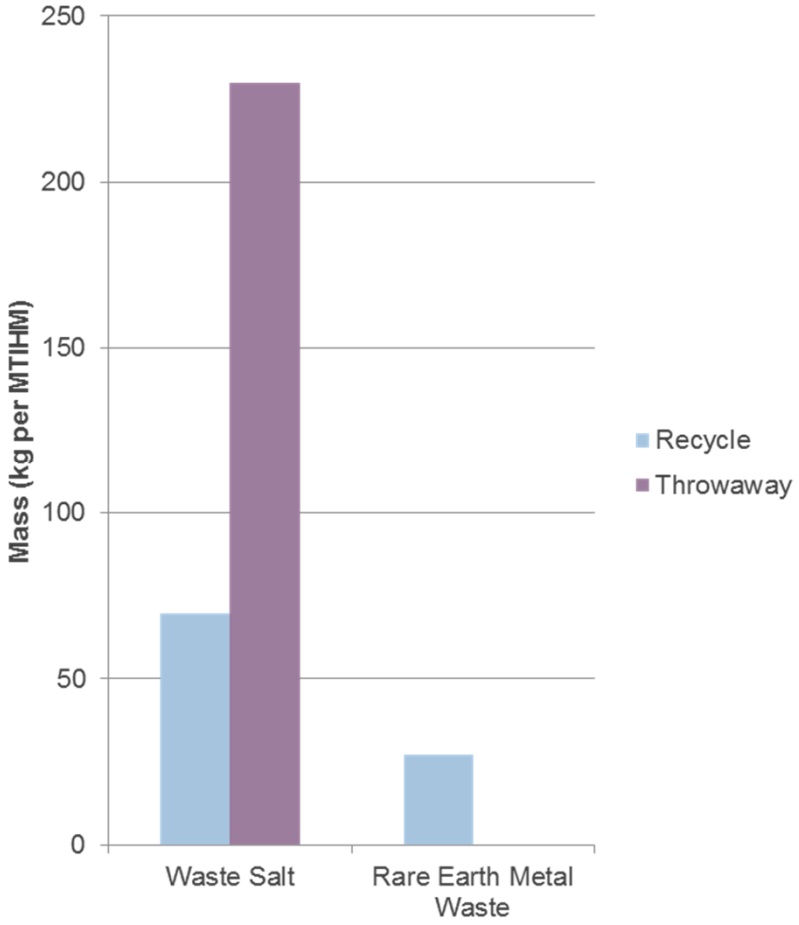


Using AMPYRE to Evaluate Flowsheet Options (Metal Fuel)



- Throwaway salt after U/TRU recovery vs. recycle after removal of rare earth and active metals
- Assumptions:
  - Max 10 wt% NaCl
  - Recycle process removes 33% NaCl and 80% CsCl and $SrCl_2$
- Salt treatment process needs to be defined

Summary of FY-2014 Modeling Activities and Future Work

- Simulated system response to changes and variations
- Developed chemistry-based models for anode and cathode subunits
- Enhanced user interface to automate tasks and provide flexibility
- Integrate dynamic electrorefiner model with mass balance facility model
- Expand dynamic subunit models
- Link in-process observables with chemical process models
  - Provide inputs to monitors and sensors
  - Improve identification of dynamic trends
  - Support development of other codes

Acknowledgements

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